## **1-Octadecanol** 112-92-5 | DTXSID8026935

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Marada I	D. L.
Model	Data
110001	Bata

# Weighted KNN model

5-fold CV (	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

### **Model Results**

Predicted value: 1.32e-08 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 5.09e-01

## Nearest Neighbors from the Training Set

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1-Octadecanol

Measured: 4.07e-09 Predicted: 1.32e-08

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Heptadecan-1-ol

Measured: 3.12e-08 Predicted: 4.13e-08

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1-Hexadecanol

Measured: 9.69e-08 Predicted: 9.67e-08

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1-Pentadecanol

Measured: 4.48e-07 Predicted: 2.58e-07

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Octadecanoic acid Measured: 2.10e-06 Predicted: 7.52e-07